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LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Model Reports
Quality Implementing Procedure ID:
OSTI-LLNL-QIP-SIII.2, Rev.0, Mod.0

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Disclaimer

MODEL REPORTS

1. PURPOSE

This Quality Implementing Procedure (QIP) establishes the responsibilities and process for the preparation, approval, and revision of Model Reports. This procedure describes the process and actions to implement the requirements of the OSTI-LLNL Quality Assurance Plan (QAP) which implements the U.S. Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) *Quality Assurance Requirements and Description* (QARD), DOE/RW-0333P. This procedure may also be used for model reports not subject to the requirements of the QAP per the direction of the Project Manager (PM).

2. SCOPE

This QIP applies to individuals within the Office of Science & Technology and International (OSTI)-Lawrence Livermore National Laboratory (LLNL) Project, and other participants who prepare model reports in support of the OSTI-LLNL activities. This procedure has been prepared in accordance with OSTI-LLNL-QIP-5.0, *Preparing the Quality Assurance Plan and Quality/Technical Implementing Procedures.*

Implementation of conceptual models into new mathematical models, or into mathematical models undergoing revision or change, must be documented in accordance with this procedure. Mathematical model development, validation, and initial use, as well as any related work required to accomplish these tasks, shall be documented within the model report.

Scientific information (such as data, analyses, interpretations or conclusions) is documented in accordance with OSTI-LLNL-QIP-SIII.1, *Technical Reports.* Development, revision, configuration management, verification/validation, and/or qualification of software are documented separately in accordance with OSTI-LLNL-QIP-SI.0, *Software Management.*

3. PROCEDURE

3.1 Planning

3.1.1 Project Manager (PM)/Deputy Project Manager (DPM) (or designee):

A. Control the development, validation, checking, documentation, revision, and change of the model activity in accordance with the requirements of this procedure. A Principal Investigator (PI) may be assigned to control these functions.

B. Review the Technical Work Plan (TWP) associated with the model to be developed. If the TWP requires revision, ensure that it is completed in accordance with OSTI-LLNL-QIP-2.2, *Planning for Science Activities.*

1. Ensure the applicable TWP includes adequate planning for model validation, including the identification of the intended purpose of the model, the needed level of confidence for the model, the criteria to be used to determine that the appropriate level of confidence has been met, the plans for independent technical review per Section 3.3, and the plans for post-development model validation activities. Planning requirements for conducting modeling are contained in OSTI-LLNL-QIP-2.2.

2. If a previously developed model is to be used outside of its intended use, limitation, or range of validity, justification and plans for validation shall be provided in the applicable TWP.

3. Ensure that adequate planning is documented for any required data qualification activities in accordance with OSTI-LLNL-QIP-SIII.4, *Qualification of Unqualified Data.*

C. Assign an Originator (if not the PI) to perform the modeling activity and provide the originator and the PI the applicable TWP.

3.2   Preparation of Model Reports

3.2.1   Originator:

A. Perform the modeling activity and associated tasks in accordance with the applicable TWP and all applicable procedures. Scientific notebooks may be used in the modeling activity in accordance with OSTI-LLNL-QIP-SIII.0, *Scientific Notebooks.*

B. Obtain a document identifier (DI) for the Model Report from the Records Coordinator in accordance with OSTI-LLNL-QIP-6.0, *Document Control.* The Document Identifier and revision number should appear on each page of the Model Report.

C. Document the modeling activity in the Model Report using the annotated outline in the Model Report Outline (Attachment 1).

D. Ensure software used to develop and perform the modeling activity and associated tasks documented in the Model Report is controlled and documented in accordance with OSTI-LLNL-QIP-SI.0, *Software Management.*

1. Document software used to develop and perform the modeling activity and associated tasks documented in the Model Report as described in Section 3 of the Model Report Outline (Attachment 1). Document that the use of the software was consistent with the intended use and within the documented validation range of the software.

2. Ensure commercial software used during the modeling activity is controlled and tracked in accordance with OSTI-LLNL-QIP-SI.0.

Data reductions, spreadsheets, and graphic presentation of data using commercial off-the-shelf software (COTS) programs (e.g., Microsoft Excel) may be used to synthesize, summarize, or graphically present data. The computation shall be documented such that the results can be reproduced and checked by hand. This software use is considered exempt from the requirements of OSTI-LLNL-QIP-SI.0 provided that adequate information is included in the documentation in accordance with the Model Report Outline (Attachment 1).

3. Software may be used prior to qualification to develop a preliminary output. Document and control the preliminary output in accordance with OSTI-LLNL-QIP-SIII.3, *Submittal and Incorporation of Data to the Technical Data Management System.* The final output shall be produced with baselined software in accordance with OSTI-LLNL-QIP-SI.0. Make a comparison between the preliminary and final outputs. If the outputs are identical, then document the comparison and update the preliminary output with the final output on the Technical Data Information Form (TDIF). If the outputs are not identical, then document the comparison and supersede the preliminary output with a new one containing the final output in accordance with OSTI-LLNL-QIP-SIII.3.

E. Select relevant inputs for developing and supporting the Model Report information, recommendations, results, and/or conclusions. Document the Model Report inputs in Section 4 of the Model Report. Ensure that the input status (e.g., qualified data, established fact, unqualified data etc.) is clearly listed.

1. Maintain traceability of unqualified data to their status as unqualified when used in the Model Report. Combining unqualified data with qualified data renders the output, calculation, table, etc., unqualified.

2. Document the qualification of unqualified data used as direct input, in accordance with OSTI-LLNL-SIII.4, *Qualification of Unqualified Data,* as described in Section 6 of the Model Report Outline (Attachment 1).

3. Data, obtained from the literature, that are not established facts and are used as direct input must be demonstrated to be suitable for the specific application. When appropriately justified, these data are considered qualified for use within the Model Report. The following factors should be considered when presenting the case that data are suitable for intended use:

   - Reliability of data source
   - Qualifications of personnel or organizations generating the data
   - Extent to which the data demonstrate the properties of interest
   - Prior uses of the data
   - Availability of corroborating data.

4. Input obtained from an OSTI or YMP product output of a cancelled or superseded document must be demonstrated to be suitable for intended use and justified within the Model Report. When appropriately justified, these inputs are considered qualified for intended use within the Model Report.

F. If using a previously validated mathematical model, obtain the appropriate model file/product output from the OSTI-LLNL Technical Data Management System (TDMS).

G. Select references necessary to support the technical basis, recommendations, results, and/or conclusions in the Model Report. All external references are to include appropriate traceability notations (e.g., Technical Information Center [TIC] catalog numbers) or be identified as readily available. Both external and readily available references can be consulted in the course of the literature review. All references shall include sufficient information to ensure traceability. Where appropriate, references presenting contradictory opinions must be identified and addressed.

H. Prepare the Model Report in sufficient detail as to purpose, method, assumptions, inputs, references, and units such that a person technically qualified in the subject can understand the document and verify its adequacy without recourse to the Originator. Present the supporting technical information in a clear and logical fashion. The information must be technically adequate, accurate, and complete. Include page numbers, figure or table numbers, or section numbers in the text citation whenever a specific statement of fact or content contained within a reference is made. Include any additional considerations not previously listed but determined to be relevant to the technical report.

I. Ensure documentation is legible and in a form suitable for reproduction, filing, and retrieval.

J. Complete the appropriate sections of the Model Report Signature Page/Change History (Attachment 2), in accordance with the instructions.

3.3 Model Validation

3.3.1 Originator:

A. Identify and document the intended purpose, and any limitations for the model as described in Section 1 of the Model Report Outline (Attachment 1).

B. Document the criteria used to determine that the needed level of confidence for the model has been met as described in Section 7 of the Model Report Outline (Attachment 1).

1. The criteria used to establish the adequacy of the scientific basis for the model must be consistent with the intended use of the model and must be justified in the documentation.

2. The criteria used to demonstrate that the model is sufficiently accurate for its intended use must be consistent with parameter uncertainties and must be justified in the documentation.

C. If validation activities are to extend beyond the documented completion of the current model, include a description of future activities that are to be completed and a justification for extending model validation in accordance with Section 7 of the Model Report Outline (Attachment 1).

D. Validate the model to the level of confidence required in accordance with the TWP and Section 3.3.3 C of this procedure.

E. Document model validation as described in Section 7 of the Model Report Outline (Attachment 1).

F. Submit draft documentation of the results of the validation activities to the Deputy PM (or designee) for review.

3.3.2 PM/DPM/PI or designee:

Assign a Technical Reviewer other than the Originator, who has adequate qualifications to have originated the Model Report and a Quality Assurance (QA) reviewer. Multiple reviewers may be assigned to review different sections of the model report. The review shall be conducted in accordance with OSTI-LLNL-QIP-6.1, *Document Review*.

3.3.3 Technical Reviewer:

The Technical Reviewer shall use the Model Review Criteria (Attachment 3) and ensure that:

A. The mathematical models are validated for their intended purpose and stated limitations, and to the required level of confidence. Validation is required for all mathematical models and their underlying conceptual models (validation is not required for conceptual models not implemented in mathematical models).

B. The validation of the mathematical model and its underlying conceptual model includes documentation of decisions or activities that are implemented to generate confidence in the model during model development, including the following:

1. Selection of input parameters and/or input data, and a discussion of how the selection process builds confidence in the model.

2. Description of calibration activities, and/or initial boundary condition runs, and/or run convergences, and a discussion of how the activity or activities build confidence in the model. Include a discussion of impacts of any run non-convergences.

3. Discussion of the impacts of uncertainties to model results.

C. The mathematical models undergo model validation activities after the model has been developed. The model validation activity/activities completed after the model has been developed shall be dependent upon and consistent with the model's intended use and required level of confidence and shall include one or more of the following, consistent with those delineated in the applicable TWP:

   1. Corroboration of model results with data acquired from the laboratory, field experiments, analog studies, or other relevant observations, not previously used to develop or calibrate the model

   2. Corroboration of results with alternative mathematical models

   3. Corroboration with information published in refereed journals or literature

   4. Peer Review (if used, an OSTI-LLNL-QIP will be developed to control the activity prior to performing the work).

   5. Technical review, planned in the applicable TWP, by reviewers independent of the development, checking, and review of the Model Report (the Originator, PM/DPM/PI, Checker, and Reviewers assigned to the model document/activity may not serve as an independent post-development model validation Technical Reviewer)

   6. Corroboration of abstraction or system model results to the results of the validated mathematical model(s) from which the abstraction or system model was derived, including corroboration with results of auxiliary analyses used to provide additional confidence in system model results.

   7. Corroboration of pre-test model predictions to data collected during subsequent, associated testing.

D. Technical review through publication in a refereed professional journal or review by an external agency, documented by the external agency, may be used to demonstrate additional confidence in the model.

3.3.4 QA Reviewer:

The QA Reviewer shall conduct a QA review to verify the Model Report contains the information required by Attachment 1 or proper justification is provided. The QA Review may be performed concurrently with Checking or

after Checking, as directed by the PM/DPM (or designee). The QA Reviewer shall ensure that quality requirements (e.g., compliance with governing procedural requirements, management directives, associated errata, condition reports, etc.) are adhered to. Additional QA review criteria may be identified on the Review Record, as deemed appropriate by the PM/DPM (or designee).

3.3.5 Originator:

A. Resolve all comments with the Technical and QA reviewers.

B. Elevate unresolved comments to the next levels of management until resolution is achieved and document the resolution.

C. Modify the original Model Report, as required, to incorporate comment resolution.

D. Submit draft Model Report to the PM/DPM/PI (or designee) for initiation of check.

3.4 Check

3.4.1 PM/DPM/PI(or designee):

Assign a Checker to check the Model Report. The Originator, or PM/DPM/PI or designee may not perform the checking function.

3.4.2 Originator:

A. Compile a Model Report check package consisting of the items identified below. Ensure that the document to be checked is marked as a Check Copy. Documents may be provided electronically (e.g., compact disk). Forward the check package to the Checker.

   1. Draft Model Report.

   2. Any pertinent background information, that is not readily available.

3.4.3 Checker:

A. Check the Model Report ensuring that:

   1. The content and output of the model are technically adequate, complete, and correct.

   2. Software, if used, is adequate for its intended use; is identified by the software tracking number, title, and revision/version number; and has been controlled and documented in accordance with OSTI-LLNL-QIP-SI.0 or (if previously developed for the YMP) with applicable YMP procedures.

3. Appropriate inputs were selected, correctly identified in the Model Report, cited, and incorporated in the modeling activity.

4. Corroborating data, models, or information is clearly identified.

5. Any assumption, data undergoing qualification per OSTI-LLNL-QIP-SIII.4, or other input values are clearly identified and justified.

6. The implications of uncertainties and restrictions are discussed and are evaluated within the Model Report.

7. The assumptions, constraints, bounds, or limits on the inputs are identified in the Model Report, and their impact on the results are described and assessed in the documentation.

8. The discussion of scientific approach and/or technical methods is documented.

9. The referencing is thorough, accurate, and complete, including appropriate tracking numbers (e.g., records accession numbers, Data Tracking Numbers [DTN] etc.).

10. Justification and model validation documentation are provided for using a previously developed model outside of its intended purpose, limitations, or range of validity.

11. Data, used as direct input are verified to their home information system/controlled source (e.g., data are verified to be the same as the ones posted on the Technical Data Management System [TDMS]).

12. Validation has been completed in accordance with the applicable TWP and the requirements of this procedure.

13. Any work performed to develop a preliminary output using software in scoping and bounding determination, feasibility studies, prototype methodology development, or similar activities, as allowed by OSTI-LLNL-QIP-SI.0, has subsequently been verified and is adequately documented per Section 3.2.1 D. A checker comment shall be made documenting that additional checking is required when the work producing the final output is documented in the Model Report.

B. Clearly and legibly write, or mark electronically, all comments on the Checker Check Copy or indicate that there are no comments. (Comments may be documented separately if keyed to the Check Copy and if comment documentation is signed, dated, and attached to the Check Copy.)

C. Initial and date the Checker Check Copy of the Model Report Signature Page/Change History (Attachment 2) and return the documentation to the Originator.

3.4.4 Originator:

A. Resolve all comments with the Checker and document the resolution by mark up of the applicable Check Copy, including the proposed resolution for accepted comments and the rationale for comments not incorporated or only partially incorporated. Initial and date each resolution. Resolution may be documented separately if keyed to the applicable Check Copy and the resolution documentation is signed, dated, and attached to the Check Copy.

B. Elevate unresolved comments to the next levels of management until resolution is achieved and document the resolution. (Resolution may be documented separately if keyed to the applicable Check Copy.)

C. Modify the original Model Report, as required, to incorporate comment resolution.

D. Denote the modified Model Report (back check) by revising the alphanumeric revision number.

E. Provide the back check copy and applicable Check Copy to the Checker.

3.4.5 Checker:

A. Check the modified Model Report by comparing it to the applicable Check Copy.

B. Indicate acceptance of the resolution of each comment, including any comment that was not incorporated or was only partially incorporated by accepting the Originator's rationale or by providing separate justification. Initial and date each acceptance. Use additional pages as necessary. Acceptance may be documented separately if keyed to the applicable Check Copy.

C. Initial and date the applicable Check Copy of the Model Report Signature Page/Change History (Attachment 2) and return the Model Report to the Originator

D. QA Reviewer review the modified Model Report to verify that incorporation of the resolution of checker comments does not violate QA requirements.

3.5 Product Output

3.5.1 Originator:

A. Submit the following key technical data to the Technical Data Coordinator for submittal to the TDMS in accordance with OSTI-LLNL-QIP-SIII.3:

   1. Product output that replaces or supersedes product output or data that are currently in the TDMS.

2. Data that have undergone a status change, as a result of a qualification within the technical report.

3. Other output may be submitted, as directed by the PI.

B. Finalize or supersede preliminary product output, if any, in accordance with OSTI-LLNL-QIP-SIII.3.

3.6 Approval of Model Reports

3.6.1 Originator:

A. Prepare the final Model Report by changing the alphanumeric designator to a numeric designator (i.e., the initial Model Report designator is "00," and subsequent revisions are "01," etc.) and updating the change history, as necessary.

B. Complete the Model Report Signature Page/Change History (Attachment 2).

C. Submit the approved document to the Records Coordinator in accordance with OSTI-LLNL-QIP-6.0.

D. Submit the Model Report records to the Records Coordinator in accordance with Section 4.0.

3.6.2 PM/DPM/PI:

If the Model Report is identified as a deliverable to DOE, submit the approved Model Report with a transmittal letter. Any changes to the Model Report resulting from DOE review comments shall follow section 3.8.

3.7 Editorial Corrections

3.7.1 Originator:

A. If the Model Report requires editorial corrections after approval but before controlled distribution, change the in-process master as follows:

1. Mark the change(s) by drawing a single line through the change(s) (i.e., pen/ink or electronic changes) and/or inserting the new or correct information.

2. Initial and date the change(s).

3. Note the change(s) in the Remarks section of the Model Report Signature Page/Change History (Attachment 2, Block 9).

B. Obtain PM's approval.

3.8 Model Report Revision, Change or Cancellation

PM/DPM/PI:

A. Determine whether the Model Report will be modified as a revision or as an Interim Change Notice (ICN). Reviews and checks of ICNs are limited to the changes and the portions of the Model Report affected by the changes.

B. When initiating a revision or change to an existing document, notify the Records Coordinator of the impending action to ensure version control.

C. Issue no more than five ICNs against a Report revision.

D. Process a revision or change in the same manner as the original, in accordance with requirements of Section 3.0. When a Model Report is revised or changed, the entire product must be brought into compliance with current versions of relevant procedures. Indicate revisions or interim changes in the Model Report using one of the following:

   1. A black vertical line in the margin of the page, and notes clearly indicating which individual sections were revised, as applicable, and a brief description of the revision or change in the Model Report Signature Page/Change History (Attachment 2, Block 12).

   2. A note in the Model Report Signature Page/Change History (Attachment 2, Block 12) indicating the entire Model Report was revised and the changes were too extensive to use vertical lines to identify revised sections

E. Address any applicable Errata, documented in accordance with OSTI-LLNL-QIP-16.0, *Condition Reporting and Resolution,* in the appropriate section of the model document. List any errata addressed in the Remarks section of the Model Report Signature Page/Change History (Attachment 2, Block 9).

F. Notify the Records Coordinator of intention to cancel Model Reports that are no longer relevant to the project in accordance with OSTI-LLNL-QIP-6.0.

3.9 Errors

Originator:

Document errors identified and processed in accordance with OSTI-LLNL-QIP-16.0 in the following manner:

1. Generate an Errata Sheet in accordance with OSTI-LLNL-QIP-16.0.

2. Submit the Errata Sheet to the Records Coordinator in accordance with OSTI-LLNL-QIP-6.0.

4. RECORDS

The records listed in Sections 4.1 and 4.2 shall be collected and submitted to the Records Coordinator in accordance with OSTI-LLNL-QIP-17.0, *Records Management*, as individual records or included in a records package, as specified. The records listed in Section 4.3 shall be dispositioned by the Records Coordinator in accordance with OSTI-LLNL-QIP-17.0.

4.1 QA Records

For a Model Report subject to the requirements of the QAP:

Records Package:

All QA records generated by OSTI-LLNL-QIP-6.1
Check Copies
Approved Model Report submitted per OSTI-LLNL-QIP-6.0

4.2 Non-QA Long-Term Records

Review Drafts.

For a Model Report not subject to the requirements of the QAP:

Records Package:

All non-QA records generated by OSTI-LLNL-QIP-6.1
Check Copies
Approved Model Report submitted per OSTI-LLNL-QIP-6.0

4.3 Non-QA Short-Term Records (three years or less retention)

Transmittal letter to DOE

5. RESPONSIBILITIES

5.1 The **PM** (or designee) is responsible for assigning the PI and Originator responsible for the development, documentation, revision, change and approval of the Model Reports and the final disposition of disputed review comments.

5.2 The **Deputy PM**, when assigned, (or designee) is responsible for appointing Technical, and QA Reviewers and Checkers for Model Reports on the basis of education, training and experience. The Deputy PM (or designee) is also responsible in assigning specific review criteria, as deemed appropriate.

5.3 The **Quality Assurance (QA) Manager** (or designee) is responsible for overseeing the preparation, change and approval of this procedure, and for providing assistance and guidance to staff members in the review process and for reviewing the Model Report for compliance with applicable OSTI-LLNL QA Program requirements.

5.4 The document **Originator** (the first or lead author) is responsible for preparing a Model Report and overseeing persons who have made material contributions to the work and composition; for accepting professional responsibility for its contents; and for completing the Model Report and scheduling and coordinating the review process.

5.5 The **Checker** is responsible for performing checks for both technical issues and compliance with procedural controls. The technical checker assigned to check a part of a Model Report shall have adequate education, training and experience to understand and evaluate the contents of the Model Report being checked. A checker shall not have participated in the authorship of the portion of the document (e.g., chapter) under his or her check.

5.6 The **Technical Reviewer,** a technically competent individual, other than the Originator and from the same technical area as the Originator, is responsible for reviewing the model report, providing written comments on the Comment Sheet or draft report, and evaluating/accepting Originator responses. Comments shall be returned to the Originator in a timely manner.

6. ACRONYMS AND DEFINITIONS

6.1 Acronyms

COTS	Commercial Off-the-Shelf Software
DI	Document Identifier
DOE	U.S. Department of Energy
DPM	Deputy Project Manager
DTN	Data Tracking Number
ICN	Interim Change Notice
LLNL	Lawrence Livermore National Laboratory
OCRWM	Office of Civilian Radioactive Waste Management
OSTI	Office of Science & Technology and International
PI	Principal Investigator
PM	Project Manager
QA	Quality Assurance
QAP	Quality Assurance Plan
QARD	Quality Assurance Requirements Description
QIP	Quality Implementing Procedure
RC	Records Center
TDIF	Technical Data Information Form
TDMS	Technical Data Management System
TIC	Technical Information Center
TWP	Technical Work Plan
YMP	Yucca Mountain Project

6.2 Definitions

Concurrence Draft: A draft of a scientific document or data set that has been revised to incorporate comments generated by Reviewer(s), and that is considered by the document/data Originator to be ready for concurrence and approval.

Direct Input: Input that are used to develop of results or conclusions in the Technical or Model Report.

Editorial Corrections: Corrections made to a document such as correcting grammar, spelling, or obvious typographical errors; renumbering sections or attachments (as long as the renumbering does not affect the chronological sequence of work); modifying the title or number of the document (as long as the fundamental process is not changed); updating organizational titles (as long as responsibilities are not changed); or making other corrections or clarifications of intent that do not alter the results or the way a document is used.

Errata: An error, discrepancy, or inconsistency in a document.

Indirect Input: Input that is used to provide additional information that is not used in the development of results or conclusions in the Technical or Model Report.

Input: A source of information or data that is used in the scientific investigation.

Governing Procedure: The document invoking implementation of a procedure.

Model: A model representation of a system, process, or phenomenon, along with any hypotheses required to describe the process or system or explain the phenomenon, often mathematically (QARD).

Originator: The first or lead author who has overall responsibility for preparing a scientific document and overseeing persons who have made material contributions to the work and composition, and who accepts professional responsibility for its contents.

Review Comment: A comment requiring resolution that identifies a problem such as a conflict with existing OCRWM requirements, failure to meet stated review criteria, or an inadequacy or error that could adversely impact the suitability of the document for its intended purpose.

Scientific Investigation: Any observation, identification, description, experimental study, or analysis and explanation of natural phenomena. (QARD)

Technical Report: As it pertains to scientific investigation, a document that presents scientific information such as data, analyses, interpretations or conclusions. (QARD)

7. REFERENCES

Quality Assurance Requirements and Description, DOE/RW-0333P

OSTI-LLNL-QIP-2.2, *Planning for Science Activities*

OSTI-LLNL-QIP-5.0, *Preparing the Quality Assurance Plan and Quality/Technical Implementing Procedures*

OSTI-LLNL-QIP-6.0, *Document Control*

OSTI-LLNL-QIP-6.1, *Document Review*

OSTI-LLNL-QIP-16.0, *Condition Reporting and Resolution*

OSTI-LLNL-QIP-17.0, *Records Management*

OSTI-LLNL-QIP-SI.0, *Software Management*

OSTI-LLNL-QIP-SIII.0, *Scientific Notebooks*

OSTI-LLNL-QIP-SIII.1, *Technical Reports*

OSTI-LLNL-QIP-SIII.3, *Submittal and Incorporation of Data to the Technical Data Management System*

OSTI-LLNL-QIP-SIII.4, *Qualification of Unqualified Data*

OSTI-LLNL-QIP-SV.0, *Management of OSTI-LLNL Electronic Data*

8. ATTACHMENTS

Attachment 1 – Model Report Outline

Attachment 2 – Model Report Signature Page/Change History

Attachment 3 – Model Report Review Criteria

9. REVISION HISTORY

2/25/05 Revision 0, Modification 0

   Initial Issue

10. APPROVALS

Preparer: Leigh Gouveia   Date: 2/25/05

Technical Reviewer: QINHONG HU   Date: 2/25/05

QA Reviewer: VICTOR J. BARISH JR   Date: 2/25/05

Project Manager: DAVID B. McCALLEN   Date: 2/25/05

MODEL REPORT OUTLINE

If any of the following sections are not applicable to a particular model, a brief statement of non-applicability is required for Report purposes under each heading. The document may include additional sections (e.g., an Executive Summary) to assist "users" of the model. Information presented in the Model Report shall be transparent and traceable.

1. **Purpose** –This section shall provide the intended use of the model, the model limitations (e.g., data available for model development, valid ranges of model application, spatial and temporal scaling), and scope of the Model Report. It shall also refer to the TWP for the activity. Document any deviation from the TWP in the appropriate section and provide justification for the deviation.

2. **Quality Assurance** – This section shall include the applicability of the QA program, including evaluation of associated activities in accordance with appropriate implementing procedures. If scientific tasks included in the Model Report activity have been determined not to be subject to the QAP, provide justification. Reference the TWP for the determination of the applicability of the QAP. If the analysis investigates an item or barrier on the Q-List, identify the item or barrier and its safety category as directed by the memorandum of *"Guidance and Funds to Lawrence Livermore National Laboratory for Tasks from the Office of Civilian Radioactive Waste Management."* This section will describe any variance from the planned method(s).

3. **Use of Software** – This section shall include a list of all controlled and baselined software as described in OSTI-LLNL-QIP-SI.0 or (if previously developed for the YMP) applicable YMP procedures. Document the use of the software, including the software name, tracking number, version, and operating environment (including platform and operating system).

    Include a list of any software that was used prior to qualification to develop a preliminary output. If the solution to the calculation or analysis package used to support this technical product is obtained using the standard functions of a commercial off-the-shelf software program (e.g., EXCEL, MATHCAD, and EARTHVISION) and the results are not dependent on the software program used, this software does not need to follow OSTI-LLNL-QIP-SI.0.

    If the results are not dependent on the software program, the actions performed (as indicated below) shall be documented in sufficient detail in this technical product to allow an independent reviewer to reproduce or verify the results by visual inspection or hand calculation without recourse to the Originator:

    *   The formula or algorithm used

    *   A listing of the inputs to the formula or algorithm

    *   A listing of the outputs from the formula or algorithm

- Other information (e.g., operating environment information) that would be required in order for any independent person to reproduce the work.

4. **Inputs** – Technical product inputs shall be correctly selected, identified in the Model Report, correctly cited and incorporated.

    4.1 Direct Input –The appropriateness of technical product inputs (data, models, or technical product output) directly used to develop the model shall be documented and substantiated in this section.

        - Provide lists or tables of inputs that were used directly in the development of the model. Identify inputs by DTN, TIC number or other applicable document identifier and indicate the qualification status (i.e., qualified data, established fact etc.)

        - If the present study uses, revises, or changes a previously developed and validated model to complete the present study, list associated DTNs, accession numbers, report titles, and document identifying numbers, if applicable.

    4.2 Criteria – List criteria that the document must satisfy as stated in the TWP, including requirements contained in applicable DOE requirement documents and any relevant acceptance or completion criteria. (Model Validation criteria should be documented in Section 7 of the model document.)

    4.3 Codes and Standards – Provide a list of the applicable codes (only if the model directly addresses federal or other code requirements) and standards (e.g., American Society for Testing and Materials or Occupational Safety and Health Administration standards) used in the model by name, number, and date, including applicable revision status, using date or revision designator.

5. **Assumptions** – This section shall include a description of the assumptions used, in the absence of direct confirming data or evidence, to perform the model activity. Assumptions shall be clearly stated and the rationale for suitability of the use of the assumption shall be included. Other model assumptions are described in Section 6 of the Model Report.

6. **Model Discussion** – Include a description of the system, process, or phenomenon conceptual model and the scientific, engineering, and mathematical concepts/principles on which the mathematical model is based. Establish the appropriateness of the model for the purposes and within the limitations stated in Section 1 of this attachment.

The use of a scientific notebook(s) in accordance with OSTI-LLNL-QIP-SIII.0, as applicable, is allowed for documenting the model activities, but final model report shall be completed to the requirements of this procedure. The Model Report can refer to the scientific notebook(s) by title, number, organization, records accession number, or similar information.

Provide lists or tables of corroborating/supporting data, models, or product output used to develop the model. Identify the sources of the corroborating/supporting information. Document the qualification of unqualified data developed in accordance with OSTI-LLNL-QIP-SIII.4. Include additional discussions to substantiate input used in this section if not included in Section 4. Address any differences in direct input values between values brought forward in Section 4 and values used in this section.

The following topics shall be included in this section, as applicable, when documenting a model:

- A detailed description of the conceptual model and the conceptual model implementation (mathematical model)

- Results of literature searches or other background information

- A discussion of uncertainties, sources of uncertainties, and impacts of uncertainties on model output

- Alternate models that were not used and the rationale for not selecting them

- Units of measurement

- Description of the input data used to generate input files for each model simulation

- A discussion of initial and/or boundary conditions

- A discussion of model assumptions (other than those made in the absence of direct confirming data or evidence), mathematical formulations, equations, algorithms, and numerical methods used.

- A discussion of the results of model testing, sensitivities, and calibration activities

- Intended use of the model output

- Comparison between the preliminary and final outputs, as applicable.

7. **Validation**–The model validation documentation shall include:

- Lists or tables of corroborating/supporting data, models, or information used to complete model validation activities. Identify the sources of the corroborating/supporting information.

- Level of model importance and required level of confidence.

- Documentation and discussion of model validation activities performed in Section 3.3 of this procedure.

- Results of the validation activities.

- Model validation criteria explicitly specified for ensuring the appropriate level of confidence has been obtained, consistent with Section 3.3 and the applicable TWP.

- Rationale for determining that the validation criteria have been met.

- Any future activities that need to be accomplished for model validation and a justification for extending model validation beyond the documented completion of the current model.

Because model validation may consist of a sequence of separate activities, each model validation activity should be documented in accordance with the requirements of this procedure upon its completion.

8. **Conclusions** – This section shall provide a summary of the modeling activity. The conclusions, including the DTNs and/or tables or lists of product output as well as any decisions or recommendations based on the modeling activity, shall be presented in this section. Conclusions shall include any uncertainties and restrictions for subsequent use. Any confirmatory actions, such as compliance runs, additional sensitivity runs, and neutralization runs, shall be addressed.

9. **Inputs and References** – Sources of inputs, software, DTNs, and cited references (including references used to justify assumptions) shall be listed in this section. Inputs and references include materials that support the conclusions of the model. These may include published reports, technical papers, scientific notebooks, literature searches, or other background information. The online Style Manual may be used as guidance on formatting reference lists and citations.

Appendices–Supporting documentation, such as computer output, that are lengthy or cannot be conveniently included within the main text of the documentation may be included as appendices. Computer output may be attached as hardcopy, read-only disk but must meet the requirements of OSTI-LLNL-QIP-17.0. Computer output files included as appendices are exempt from page numbering, DI, and revision number requirements provided the total number of pages in each appendix (for hardcopy) or complete file information, including all file names, file dates and times, and file sizes, are documented on the appendix. In case of printed appendices, the total page count for each appendix shall be documented on the Model Report Signature Page/Change History (Attachment 2). Where the appendix is on computer media, the quantity and type of media shall be clearly identified on the Model Report Signature Page/Change History (Attachment 2).

Lawrence Livermore National Laboratory	**OSTI-LLNL** **MODEL REPORT SIGNATURE PAGE/ CHANGE HISTORY**	1. Page of

2. Model Report Title			
3. DI (Including Revision Number)			
4. Total Appendices		5. Number of Pages in Each Appendix	
	Printed Name	Signature	Date
6. Originator			
7. Checker			
8. Project Manager			
9. Remarks			

<div align="center">CHANGE HISTORY</div>

10. Revision No.	11. Total pages	12. Description of Change

INSTRUCTIONS FOR MODEL REPORT SIGNATURE PAGE/CHANGE HISTORY

Originator

1. Enter the total number of pages (excluding appendices).

2. Enter the title of the Model Report.

3. Enter the DI, including revision number and change number, if applicable.

4. Indicate the total number of appendices.

5. Indicate the number of pages in each appendix (e.g., A-11, B-5, and C-20). Computer output may be included as hardcopy or as electronic data files contained on appropriate media. In the case of printed appendices, document the total page count for each appendix. If the appendix is on computer media, identify the quantity and type of media attached. If necessary, this information may be placed in Block 9, Remarks, with a reference to Block 5.

6. Print or type name; sign and date.

Checker

7. Print or type name; sign and date when all comments have been resolved and changes have been incorporated into the Model Report.

Project Manager

8. Print or type name; sign and date to signify approval.

PI/Originator, Checker, Project Manager

9. Include remarks or supplemental information on appendices from Block 5, if required. Indicate any other limitations on the use of the model. The Remarks section of the review copy may also be used to document those draft documents that are in concurrent review and that were used as input.

Originator

10. Identify any revisions or ICNs to this Model Report, in order, starting with Rev 00 and continuing to the latest revision/ICN.

11. Enter the total page count, including appendices and cover, for each revision/ICN.

12. For any revisions or ICNs to this Model Report, enter a brief description of each change and the reason for the change (e.g., "added Appendices A and B").

MODEL REPORT REVIEW CRITERIA

1. Does the Model Report present a clear introductory statement of the technical purpose, scope, and objectives?

2. Input Data:

   a) Are the input data adequately described in the Model Report?
   b) Is this discussion sufficient to demonstrate that these data were used properly to perform the modeling activity?
   c) Does the Model Report adequately document the use and interpretation of these data, including effects and consequences of data limitations?

3. Is the level of detail and manner of presentation, including tables and figures, sufficient to allow a technically qualified individual to understand the development of the technical arguments, the scientific and mathematical methods used, the conclusions reached, and the presentation of technical information and results without recourse to the Model Report originator?

4. Are the technical arguments sound and appropriate and adequate to support the results and conclusions?

5. Are the technical assumptions identified and are adequate bases for these assumptions provided?

6. Is there adequate discussion of the scientific and mathematical methods and model(s) that are used together with the rationale for the selection of these methods or model(s)?

7. Is there adequate discussion of alternative models, methods, and approaches?

8. Are the model range of applicability, the model limitations, and the model uncertainty and its consequences addressed adequately?

9. Does the Model Report demonstrate that the modeling activity is appropriate and adequate for its intended purpose, or, alternatively, does the Model Report describe appropriate methods or approaches that will be used to address model validation?

10. If the Model Report also documents an analysis, does the report describe the limitations of the analysis and provide a technically adequate discussion of precision, accuracy, and representativeness of results?